Quasirelativistic calculation of $4s^24p^5$, $4s^24p^44d$ and $4s4p^6$ configuration spectroscopic parameters for the W^{39+} ion

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Abstract.

The *ab initio* quasirelativistic Hartree-Fock method developed specifically for the calculation of spectral parameters of heavy atoms and highly charged ions is used to derive spectral data for the 4s²4p⁵, 4s²4p⁴4d and 4s4p⁶ configurations of the multicharged tungsten ion W³⁹⁺. The relativistic effects are taken into account in the Breit-Pauli approximation for the quasirelativistic Hartree-Fock radial orbitals. The configuration interaction method is applied to include the electron correlation effects. Produced data are compared with existing experimental measurements and theoretical calculations.

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1. Introduction

Metallic tungsten is becoming one of the popular materials in high-temperature devices, including fusion reactors [1,2]. The tungsten material is difficult to vaporize. Nevertheless, the highly-charged ions of tungsten can emerge in fusion plasma causing the decrease of its temperature. Thus there is a need to control the concentration of these ions by monitoring their spectra. Only reliable theoretical data of the multicharged tungsten ion spectral properties enable to model such types of plasma providing means to its diagnostics, see e.g. [3]. On the other hand, the theoretical energy spectra and transition parameter calculations are helpful in identifying the emission lines of the multicharged tungsten ions which are observed in the specially designed experiments.

This situation has increased interest from both the experimental and theoretical physicists in study of the tungsten ions of various ionization stages. An extensive compilation of the experimental data and their semi-empirical investigation has been reported in [4]. A consequent review of the experimental and theoretical works is reported in [5]. Over the last few years, several experimental works (see, e.g. [6–9] and the references therein) on the tungsten ions are published. Alongside there is a considerable interest in multicharged ions from theoreticians. Some part of reported calculations are based on different variational methods utilizing the solutions of Dirac-Fock relativistic equations, see [10–13]. Another part of calculations [14, 15] is mainly based on the relativistic many-body perturbation theory (RMBPT) with additional calculations in [15] performed using a quasirelativistic Hartree-Fock with the superposition of configurations and the relativistic multiconfiguration Hebrew University Lawrence Livermore Atomic Code (HULLAC). A quasirelativistic approximation (QR) developed at Vilnius University was successfully applied for the study of tungsten ions in [16–18]. The above works were devoted to the tungsten ions with an open 4d shell.

The quasirelativistic investigation of the tungsten ions with an open 4d shell [16–18] has demonstrated that our QR [19–21] is capable of producing reliable and highly-accurate spectroscopic parameters for the tungsten ions of such a high ionization degree. This conclusion gives us confidence to consider the higher ionization stages and to start investigation of the tungsten ions with an open 4p shell.

In the current work we present the results for the W³⁹⁺ ion in the ground and the lowest two excited configurations. The relevance and actuality of the spectroscopic data for this ion is reflected in number of papers; for us new theoretical transition data open a way to compare those data to our calculation results and to assess the accuracy of determined spectroscopic parameters.

The experimental electron-beam-ion-trap (EBIT) measurements for the multicharged ions with an open 4p shell were reported in [22]. There authors employed theoretical data from [23] for the line identification. The fully relativistic parametric potential code RELAC [24] was adopted in [23] for the data production. Later on, some new lines of the W³⁹⁺ ion were presented in [25] where the HULLAC [26] code, analogous to the RELAC one, was used in calculations. The EBIT measurements in [27] made it possible to identify few more lines by applying the Flexible Atomic Code (FAC) [28]. Those experimental studies were summarized in [4], and the atomic data could be found in database [29].

Very recently, several new theoretical studies were reported. In those works data for the ion W^{39+} ground and two lowest excited configuration level energies, the level radiative lifetimes τ and the electron transition parameters were presented. Their studies were using fully relativistic calculations with the configuration interaction (CI) approximation used to include electron-correlation effects as implemented in the computer code GRASP (General-purpose Relativistic Atomic Structure Package) [30]. The theoretical energy levels of the ground $4p^N$ and $4d^N$ configurations of the tungsten ions and the radiative transition parameters among their levels were calculated in [10]. The data for the excited configurations of the W^{39+} were reported quite recently. The first calculation [31] results were substantially analyzed and strongly criticized in [32]. Based on the latter, the same authors presented more extensive calculation results for the W^{39+} in [33]. The discussion about the relativistic calculation of the spectral parameters [34] was extended in [35], where several systematic calculations of the W^{39+} were performed using different CI wavefunction expansions.

Our previous quasirelativistic calculations of the spectroscopic parameters for the tungsten ions with open 4d shell [16–18] pointed out to the high-accuracy of our transition probability values and their nice agreement with relativistic calculation results from [10] when the transitions among the the ground configuration levels were considered. Unfortunately, the lack of calculated data did not allow to compare data for the transitions from the levels of the excited configurations. Above mentioned W³⁹⁺ studies [33, 35] provided us with an impetus to perform a large-scale comparison of quasirelativistic and relativistic calculation data. In the next section we give a short description of employed quasirelativistic approach. In section 3 we compare our results with the data from other authors. The summary and conclusions are presented in section 4.

2. Description of quasirelativistic calculation

The quasirelativistic calculations are performed according to the description given in our previous papers [16–18] and the references therein. At the first stage, we solve the QR equations for the ground configuration $4s^24p^5$, see [19, 20]. Here we need to mention some peculiarities of our calculations. It was demonstrated in [20] that, for the averaging of QR equations over the one-electron angular momenta j, one has to improve their accuracy at the spherical r-coordinate origin ($r \to 0$) by accounting for the spin-orbit interaction. For that purpose, an additional parameter X_{np} has been introduced. The calculations for the tungsten ions with open np shell demonstrated that the X_{np} value significantly influences the values of the spin-orbit interaction parameter $\eta(4p)$. In order to improve the accuracy of the spin-orbit interaction, we have increased the parameter X_{np} value by few tens of percent compared to that in [20].

At the second step, we solve the QR equations for the 4d and 4f radial orbitals (RO) in a frozen-core potential. In order to perform our calculations in a multiconfiguration approximation, the basis of determined RO is supplemented with the transformed radial orbitals (TRO), which have variable parameters [21]. The TRO are determined for the radial orbitals having the principal quantum number $5 \le n \le 10$ and for all possible values of the orbital quantum number l, i.e. $l \le 9$.

The relativistic corrections are included in the Breit-Pauli approach specially adopted for the quasirelativistic RO [21]. We employ the same RO basis both for the even and the odd configurations. Therefore we can avoid any inaccuracies of the calculated transition parameters occurring when the non-orthogonal RO are used.

The set of the admixed configurations for the CI expansion was generated by virtually exciting one or two electrons from the external 4l shell and the internal 3l shell of the adjusted configurations $4s^24p^5$, $4s^24p^44d$ and $4s4p^6$. Such a set enables us to include comprehensively the correlation effects including the core-polarization effect. By applying this method and the generated RO basis for the ground (odd) configuration $4s^24p^5$, we can determine the total amount $M_o = 3172$ of the admixed configurations which can interact with the adjusted configuration. Further we apply the selection method for the admixed configurations. More details on this method are given in [36]. We need to mention that this method has been applied in all our previously described calculations. In the present calculation, we select $S_o = 188$ strongly-interacting configurations according to their weights in CI expansion, including the adjusted one. They produce total number of $C_o = 116008$ configuration state functions (CSF). The C_o is further reduced to $R_o = 2824$ by applying the CSF reduction methods described in [37].

For the excited (even) configurations $4\mathrm{s}^24\mathrm{p}^44\mathrm{d}$ and $4\mathrm{s}4\mathrm{p}^6$, one can generate $M_\mathrm{e}=7286$ admixed configurations. Our selection methods help us to reduce this number to $S_\mathrm{e}=949$ most important configurations. Furthermore, the initial number of CSF $C_\mathrm{e}=6234470$ is reduced to $R_\mathrm{e}=426816$ in the same way as it is done for odd configurations.

After the two-step selection methods are applied, the determined sets of CSF are employed to compute the level energies of the W³⁹⁺ ion. In our calculations, the main limiting factor is the number of the same LS terms. It determines the size of the Hamiltonian matrices to be diagonalized. In our case of the W³⁹⁺ ion, the largest number, 71039, arises for the ²F term of the even configurations. This number is close to our present computational limit. All our calculations are starting from the non-relativistic LS-coupling. After the level energies and their eigenfunctions are determined, these are adopted to calculate the spectroscopic parameters of the radiative transitions. From these data, the level radiative lifetimes are derived. During the investigation of the multicharged tungsten ions in [16, 17] we have noticed that the radiative lifetimes τ of some metastable levels can be affected by the M2 and E3 transitions to the ground configurations - not only by the M1 and E2 transitions among the levels of the excited configurations. Therefore we also have calculated such

Table 1. The level energies E (in 100 cm⁻¹) of W³⁹⁺ and the main contributions to their wavefunctions 9in %) from QR calculations.

| \overline{N} | Configuration | J | % | NIST [29] | Exp [22] | Exp [25] | QR | RELAC [22] | MCDF [33] | GK _{CV} [35] |
|----------------|----------------------------------|-----|----|--------------|----------|----------|-------|------------|--------------|-----------------------|
| 1 | $4s^24p^5\ ^2P$ | 1.5 | | | L J | [-] | 0 | 0 | 0 | 0 |
| 2 | $4s^{2}4p^{5}$ ² P | 0.5 | | 7422 | | | 7420 | 7486 | 7461 | 7474 |
| 3 | $4s^24p^4(^3P)4d^4D$ | 1.5 | 37 | | | | | 12178 | 12357 | 12165 |
| 4 | $4s^24p^4(^3P)4d^4P$ | 0.5 | 45 | | | | | 12377 | 12545 | 12347 |
| 5 | $4s^24p^4(^3P)4d^4D$ | 2.5 | 44 | 12322 | 12322 | | | 12362 | 12540 | 12353 |
| 6 | $4s^24p^4(^3P)4d^4F$ | 3.5 | | 12520 | | | | 12577 | 12745 | 12572 |
| 7 | $4s^24p^4(^1S)4d^2D$ | 1.5 | 54 | | | | 13255 | 13266 | 13337 | 13221 |
| 8 | $4s^24p^4(^3P)4d^4D$ | 3.5 | 41 | 13754 | | | 13749 | 13816 | 13992 | 13810 |
| 9 | $4s^24p^4(^3P)4d^2P$ | 0.5 | 34 | | | | 13758 | 13886 | 14066 | 13855 |
| 10 | $4s^24p^4(^3P)4d^4F$ | 4.5 | 68 | 13811 | | | 13850 | 13893 | 14063 | 13916 |
| 11 | $4s^24p^4(^1S)4d^2D$ | 2.5 | 45 | | | | 14889 | 15006 | 15083 | 14948 |
| 12 | $4s^24p^4(^3P)4d^4P$ | 1.5 | 24 | 15231 | 15231 | 15201 | 15262 | 15406 | 15468 | 15287 |
| 13 | $4s^24p^4(^3P)4d^2D$ | 2.5 | 22 | 15465 | 15465 | 15446 | 15513 | 15655 | 15723 | 15524 |
| 14 | $4s4p^6$ ² S | 0.5 | 67 | 16380 | 16380 | | 16268 | 16560 | 16867 | 16470 |
| 15 | $4s^24p^4(^3P)4d^4D$ | 0.5 | 78 | | | | 19073 | | 19395 | 19203 |
| 16 | $4s^24p^4(^3P)4d^4D_a$ | 1.5 | 34 | | | | 19458 | | 19790 | 19598 |
| 17 | $4s^24p^4(^3P)4d^4F$ | 2.5 | 45 | | 19739 | | 19809 | 19996 | 20126 | 19952 |
| 18 | $4s^24p^4(^1D)4d$ 2G | 3.5 | 59 | | | | 19900 | | 20203 | 20040 |
| 19 | $4s^24p^4(^3P)4d^4D_a$ | 3.5 | 42 | | | | 20814 | | 21221 | 21049 |
| 20 | $4s^24p^4(^1D)4d^2P$ | 1.5 | 47 | | | | 21080 | 21406 | 21510 | 21309 |
| 21 | $4s^24p^4(^1D)4d$ ² S | 0.5 | 42 | 21355 | 21355 | | 21196 | 21707 | 21759 | 21418 |
| 22 | $4s^24p^4(^3P)4d^2D_a$ | 2.5 | 31 | 21355 | 21355 | | 21239 | 21599 | 21678 | 21433 |
| 23 | $4s^24p^4(^3P)4d^2P$ | 1.5 | 43 | 21355 | 21355 | 21363 | | 21654 | 21683 | 21467 |
| 24 | $4s^24p^4(^3P)4d^2F$ | 2.5 | 43 | | | | | 21651 | 21745 | 21540 |
| 25 | $4s^24p^4(^1D)4d$ 2G | 4.5 | 68 | | | | | 21597 | 21726 | 21570 |
| 26 | $4s^24p^4(^1D)4d^2D$ | 2.5 | 29 | | 21761 | | | 21897 | 22026 | 21803 |
| 27 | $4s^24p^4(^1D)4d^2F$ | 3.5 | 56 | | | | 21887 | | 22349 | 22136 |
| 28 | $4s^24p^4(^3P)4d^2D$ | 1.5 | 39 | | | | | 23462 | 23475 | 23240 |
| 29 | $4s^24p^4(^3P)4d^2P_a$ | 0.5 | 36 | | | | | 24025 | 23947 | 23701 |
| 30 | $4s^24p^4(^1S)4d^2D_a$ | 1.5 | 34 | | | | 28316 | | 28844 | 28682 |
| 31 | $4s^24p^4(^1S)4d^2D_a$ | 2.5 | 37 | | | | 28939 | | 29515 | 29365 |
| | $MSD_{[29]}$ | | | | | | 73 | 164 | 276 | 75 |
| | $MSD_{[22]}$ | | | | | | 103 | 202 | 298 | 97 |
| | $MSD_{[25]}$ | | | | | | 82 | 206 | 259 | 73 |

transitions for the W^{39+} ion.

To perform our calculations, we have employed our own original computer codes together with the codes [38–40] which have been specifically adapted for our computing needs. The code from [38] was updated according to the methods presented in [41,42].

3. Results and discussion

The calculated level energies are presented in table 1. The level indices, total

angular momenta J, configurations and LS terms are also given in table 1. Presented percentage contributions of the LS terms are further applied to make level assignment. The term identification is rather rough and formal; it is executed according to the largest weight in the CI wavefunction expansion. Therefore, for some levels with the same total angular momentum J, the same LS-term is attributed. In these instances, the LS term has additional index "a". The duplication of term assignments is not unusual for the multicharged ions as the LS-coupling is not good enough for highly-charged ions.

Along with our QR results, we present the data from the NIST database [29] which are the same as in [4]. The experimental level energies determined from the experimental transition wavelengths given in [22, 25] are also presented. As we have mentioned in section 1, one can find results of different accuracy for the W³⁹⁺ ion. In order to make table 1 as concise as possible, we include the theoretical results only from [23, 33, 35]. Level energies in [23] were determined using the relativistic parametric potential code RELAC. Unfortunately, the list of presented energy levels is not complete for the configurations considered here. The level energies from [33] almost completely correspond to the GRASP3 results from [32]. The GK_{CV} results are taken from [35]. These data are produced using the largest CI expansion and are the closest to the experimental level energies.

All the levels are presented according to the QR energy increasing order. Such an ordering completely agrees with that of GK_{CV} results from [35] and also corresponds to the order of the experimental data. We must underline that, for the group of three levels with the same calculated energies, we assign the level numbers 21, 22, and 23. The same assignment have been done in [35], whereas the level J=2.5 from that group was given the level number 25 in [32]. As it is highlighted in [35], the ordering of some energy levels given in [23, 33] does not correspond to the ordering following from the most accurate results in [35]. Consequently, it does not correspond to the QR results. We mark those levels in the bold case in table 1. At the end of this table, we present the mean-square-deviations (MSD) determined by formula:

$$MSD = \left(\frac{\sum_{N} (E_{N}^{\text{th}} - E_{N}^{\text{exp}})^{2} (2J_{N} + 1)}{\sum_{N} (2J_{N} + 1)}\right)^{1/2}.$$
 (1)

Since several works give different sets of energy levels and slightly different energy values, we determine the MSD for each set of the experimental level energies. These MSD are distinguished by different indices. As one can clearly see, the QR results are more accurate compared to those from [22] and [33]; their accuracy is almost the same as that of GK_{CV} results from [35]. We must admit, that such an accuracy is achieved by applying significantly large CI wavefunction expansion compared to the expansion adopted in [35]. This is caused by the fact that our calculations employ the basis of the quasirelativistic RO, whereas the Dirac-Fock equation solutions are used in [35] and other mentioned theoretical studies. Moreover, the same RO basis is employed both for even-parity configurations and for those of odd parity. Therefore an additional correlation inclusion is necessary. So the CI expansion where the CSFs with

the same parity and principal quantum numbers are included (GK₂ in [35]) produces $MSD_{[29]} = 9400 \,\mathrm{cm}^{-1}$ whereas our QR calculation with the same expansion produces only $MSD_{[29]} = 35900 \,\mathrm{cm}^{-1}$.

A very nice agreement is evident when we compare our QR percentage contributions from table 1 to analogous data from the table 2 in [35]. Almost all contributions agree within 1%, only for the levels 14, 20, 23, and 26 the deviations reach 2%. Usually the QR percentage contributions are slightly lower compared to those of GK_{CV} from [35]. This happens because the larger CI wavefunction expansion is employed in our calculation.

In general, this kind of agreement of the QR and GK_{CV} results is very encouraging as calculations are performed using basically different approximations. Likewise in QR results, GK_{CV} calculations produce above-mentioned levels with the same main percentage contributions in the LS coupling and their level assignement matches that of our QR data. When we compare the QR percentage contributions to those from [33], their agreement is nice also for most levels. The differences of 1-2% can be observed not only for the largest (main) contributions but also for the other most important components of eigenfunctions. We do not present these contributions in the present work. The large deviations up to 6% between the QR results and the data from [33] are observed for the levels 20-23, and for 26. Furthermore, similar large deviations of the percentage contributions for these levels appear when the data from [33] and [35] are compared. It must be underlined, that energy ordering for these levels given in [33] does not correspond to that of QR or GK_{CV} calculations.

To determine the spectroscopic parameters in the QR approach, we have calculated the E1, M2 and E3 radiative transition data for the transitions between the levels of different-parity configurations. The M1 and E2 radiative transitions have been calculated between the levels of the same-parity configurations. Calculated radiative transition data are used to determine the lifetimes τ of the excited levels. These data are available from table 2 where the level indices correspond to those in table 1. The total angular momenta J of the corresponding levels are also given.

In this table we compare the results of our quasirelativistic calculations with the data from [33]. The agreement is really nice for most levels. The values $\tau_{[33]}$ which differ from the τ_{QR} values by more than 20% are marked in bold face. In most cases, it happens for the values where the radiative lifetimes are relatively large. As in the case of the energy spectra, the radiative lifetimes from [33] agree very well with those from [32] determined in the GRASP3 approximation. One can notice only one substantial difference. The levels 22 and 24 with J=2.5 are swapped around in [33] compared to their positions in [32]. This change makes the agreement with the QR results significantly better. Nevertheless, substantial differences between our QR data and those from [33] still exists for the levels 11 and 24.

One more point has to be underlined when one discusses the radiative lifetimes. As it is already demonstrated in [33], there exists number of levels arising from the odd-parity configurations $4s^24p^34d^2$, $4s4p^5$, and $4s^24p^4$ which are located below two high-lying even-parity levels 30 and 31. The radiative transitions to those odd-parity

Table 2. The radiative lifetimes (in ns) of the W³⁹⁺ levels.

| \overline{N} | J | QR | MCDF[33] |
|----------------|-----|----------------------|----------------------|
| 2 | 0.5 | 1.30E+2 | 1.31E+2 |
| 3 | 1.5 | 3.97E - 1 | $3.22E{-1}$ |
| 4 | 0.5 | $8.79\mathrm{E}{-2}$ | $7.15\mathrm{E}{-2}$ |
| 5 | 2.5 | $7.85\mathrm{E}{-1}$ | $6.34E{-1}$ |
| 6 | 3.5 | $3.70\mathrm{E}{+6}$ | $\mathbf{4.76E}{+6}$ |
| 7 | 1.5 | $4.71\mathrm{E}{+0}$ | $\mathbf{2.68E}{+0}$ |
| 8 | 3.5 | $2.66\mathrm{E}{+4}$ | 2.24E+4 |
| 9 | 0.5 | $2.00\mathrm{E}{-1}$ | 1.04E - 1 |
| 10 | 4.5 | $4.37\mathrm{E}{+4}$ | 3.70E + 4 |
| 11 | 2.5 | $8.40\mathrm{E}{+2}$ | $3.06\mathrm{E}{-1}$ |
| 12 | 1.5 | $2.56\mathrm{E}{-3}$ | $2.36E{-3}$ |
| 13 | 2.5 | $1.86\mathrm{E}{-3}$ | 1.75E - 3 |
| 14 | 0.5 | $1.62\mathrm{E}{-3}$ | $1.66E{-3}$ |
| 15 | 0.5 | $1.19E{-1}$ | $1.22E{-1}$ |
| 16 | 1.5 | $5.63\mathrm{E}{-1}$ | $5.11E{-1}$ |
| 17 | 2.5 | $2.36\mathrm{E}{-2}$ | 2.07E - 2 |
| 18 | 3.5 | $2.72\mathrm{E}{+2}$ | 2.60E + 2 |
| 19 | 3.5 | $1.45\mathrm{E}{+2}$ | 1.36E + 2 |
| 20 | 1.5 | $2.83\mathrm{E}{-3}$ | 1.32E - 3 |
| 21 | 0.5 | $4.19\mathrm{E}{-4}$ | 3.71E-4 |
| 22 | 2.5 | $5.42\mathrm{E}{-4}$ | 5.21E-4 |
| 23 | 1.5 | 7.29E-4 | $1.00\mathrm{E}{-3}$ |
| 24 | 2.5 | $2.23\mathrm{E}{+1}$ | $1.73\mathrm{E}{-2}$ |
| 25 | 4.5 | $2.58\mathrm{E}{+2}$ | $2.45\mathrm{E}{+2}$ |
| 26 | 2.5 | $9.42\mathrm{E}{-3}$ | $1.66E{-2}$ |
| 27 | 3.5 | $2.18\mathrm{E}{+2}$ | $2.05\mathrm{E}{+2}$ |
| 28 | 1.5 | $1.33\mathrm{E}{-3}$ | $1.22E{-3}$ |
| 29 | 0.5 | $8.16\mathrm{E}{-4}$ | $7.44E{-4}$ |
| 30 | 1.5 | $6.55\mathrm{E}{-4}$ | $6.22E{-4}$ |
| 31 | 2.5 | 7.53E - 1 | 4.37E-1 |

levels were not calculated in the present work. They were not presented in [33] also. We have to mention that the transition energies for those transitions are relatively small therefore corresponding transition probabilities can not be large. Nevertheless, determined radiative lifetimes $\tau_{\rm QR}$ are probably slightly overestimated.

In table 3 we present the radiative transition parameters for all excited levels of the W³⁹⁺ ion configurations $4s^24p^5$, $4s^24p^44d$ and $4s4p^6$. We present only those radiative transitions probabilities A which play an important role in determining the level radiative lifetimes τ .

The initial and the final level indices from table 1 and the radiative transition type are given to describe a particular transition. We compare our determined transition probabilities A_{QR} with the data from [35] calculated in the GK_2 and GK_{CV} approximations and with the transition probabilities from [33].

Table 3. The W³⁹⁺ emission transition probabilities A (in s⁻¹) determined in QR and several relativistic approximations and the percentage deviations k (see Eq.(2)).

| | | | QR | $ \begin{array}{c} MCDF \\ GK_2[35] \end{array} $ | $\frac{\text{MCDF}}{\text{GK}_{\text{CV}}[35]}$ | MCDF GRASP[33] | k |
|---|----------------|--------------------------|------------------------|---|---|------------------------|--------------------------------|
| 2 | 1 | M1 | 7.33(06) | | | 7.29(06) | -1% |
| 2 | 1 | E2 | 3.40(05) | | | 3.28(05) | -4% |
| 3 | 1 | E1 | 2.52(09) | | | 3.10(09) | 23% |
| 4 | 1 | E1 | 1.12(10) | 1 51(00) | 1 49(00) | 1.38(10) | 23% |
| 5 6 | 1 1 | E1 M2 | $1.27(09) \\ 1.51(02)$ | 1.51(09) | 1.42(09) | $1.58(09) \\ 1.41(02)$ | 24% -7% |
| 6 | 5 | M1 | 9.06(01) | | | 6.89(01) | -24% |
| 6 | 1 | E3 | 2.84(01) | | | (-) | |
| 7 | 1 | E1 | 2.03(08) | | | 3.61(08) | 78% |
| 7 | 2 5 | E1 M1 | 9.65(06) | | | 1.24(07) | $\frac{29\%}{21\%}$ |
| 8 | 1 | M2 | $2.04(04) \\ 1.06(04)$ | | | $2.46(04) \\ 1.18(04)$ | $\frac{21}{11}$ % |
| 8 | 6 | M1 | 6.63(03) | | | 8.38(03) | 26% |
| 9 | 1 | E1 | 3.41(09) | | | 8.44(09) | 148% |
| 9 | 2 | E1 | 1.59(09) | | | 1.18(09) | -26% |
| 10 | 6 | M1 | 2.29(04) | | | 2.70(04) | 18% $2.9 \cdot 10^5\%$ |
| 11 11 | 1 7 | E1 M1 | 1.12(06) $4.28(04)$ | | | $3.27(09) \\ 5.60(04)$ | 31% |
| 12 | 1 | E1 | 3.90(11) | 4.10(11) | 3.99(11) | 4.24(11) | 9% |
| 13 | 1 | E1 | 5.39(11) | 5.67(11) | 5.53(11) | 5.71(11) | 6% |
| 14 | 1 | E1 | 5.91(11) | 6.17(11) | 6.03(11) | 5.78(11) | -2% |
| 14 | 2 | E1 | 2.65(10) | | | 2.55(10) | -3% |
| 15 15 | $\frac{1}{2}$ | E1 E1 | 6.57(09) 1.84(09) | | | $6.47(09) \\ 1.72(09)$ | -2% -6% |
| 16 | $\frac{2}{2}$ | E1 | 1.66(09) | | | 1.60(09) | -4% |
| 16 | $\overline{1}$ | $\overline{\mathrm{E1}}$ | 1.14(08) | | | 3.53(08) | 210% |
| 17 | 1 | E1 | 4.24(10) | 3.99(10) | 4.03(10) | 4.84(10) | 14% |
| 18 | 6 | M1 | 2.87(06) | | | 3.00(06) | 5% |
| 18 18 | $\frac{5}{6}$ | M1 E2 | 4.66(05) $1.26(05)$ | | | $4.81(05) \\ 1.34(05)$ | 3% $7%$ |
| 19 | 10 | M1 | 2.77(06) | | | 2.95(06) | $\frac{1}{7}\%$ |
| 19 | 8 | M1 | 1.99(06) | | | 2.08(06) | 4% |
| 19 | 13 | M1 | 1.29(06) | | | 1.28(06) | -1% |
| 19 | 11 | M1 | 4.97(05) | | | 7.02(05) | 41% |
| 19 19 | 5 10 | M1 E2 | 1.28(05) $9.66(04)$ | | | $1.35(05) \\ 1.06(05)$ | $6\% \\ 10\%$ |
| 20 | 10 | E1 | 3.54(11) | 3.57(11) | 5.18(11) | 7.60(11) | 115% |
| 21 | 1 | E1 | 2.38(12) | 2.49(12) | 2.42(12) | 2.69(12) | 13% |
| 22 | 1 | E1 | 1.85(12) | 1.97(12) | 1.86(12) | 1.92(12) | 4% |
| 23 | 1 | E1 | 1.37(12) | 1.46(12) | 1.18(12) | 9.91(11) | -28% |
| $\begin{array}{c} 24 \\ 24 \end{array}$ | 1 8 | E1 M1 | $3.79(07) \\ 4.56(06)$ | | | $5.78(10) \\ 4.80(06)$ | $\frac{1.5 \cdot 10^5\%}{5\%}$ |
| $\frac{24}{24}$ | 11 | M1 | 2.09(06) | | | 2.10(06) | 0% |
| 25 | 10 | M1 | 2.91(06) | | | 3.06(06) | 5% |
| 25 | 8 | M1 | 6.68(05) | | | 7.05(05) | 5% |
| 25 | 10 | E2 | 1.25(05) | | | 1.36(05) | 8% |
| $\begin{array}{c} 25 \\ 26 \end{array}$ | 8 | E2 E1 | 8.56(04) $1.06(11)$ | 1.13(11) | 7.78(10) | $3.39(04) \\ 6.01(10)$ | -60% -43% |
| $\frac{20}{27}$ | 10 | M1 | 2.55(06) | 1.10(11) | 1.10(10) | 2.67(06) | 5% |
| 27 | 8 | M1 | 8.18(05) | | | 8.80(05) | 8% |
| 27 | 11 | M1 | 6.49(05) | | | 6.24(05) | -4% |
| 27 27 | 13 11 | M1 E2 | 2.21(05) | | | $3.12(05) \\ 1.04(05)$ | $\frac{41\%}{10\%}$ |
| $\frac{27}{27}$ | 10 | E_2 | 9.49(04) $8.62(04)$ | | | 9.85(04) | 10% $14%$ |
| $\frac{21}{27}$ | 17 | M1 | 5.30(04) | | | 6.42(04) | 21% |
| 28 | 2 | E1 | 6.59(11) | | | 6.98(11) | 6% |
| 28 | 1 | E1 | 9.41(10) | | | 1.19(11) | 26% |
| 29 29 | 2 1 | E1 E1 | $1.21(12) \\ 1.14(10)$ | | | $1.34(12) \\ 1.62(09)$ | 10% -86% |
| $\frac{29}{30}$ | 2 | E_1 | 1.53(12) | | | 1.62(09) $1.61(12)$ | -80 % 5% |
| 31 | $\bar{1}$ | $\overline{\mathrm{E1}}$ | 1.31(09) | | | 2.27(09) | 73% |

It is worth mentioning that inclusion of the 3d-shell polarization, which corresponds transition from the approximation GK_2 to the GK_{CV} in [35], makes the agreement of QR results and the latter data better for most transitions.

The transition probability values in the GK_{CV} approximation agree with our QR data within few percent limits for more than half of considered lines. The main exclusions from that path are the radiative transitions from the levels 20 and 26 to the lowest level 1. In this case, the inclusion of the 3d-shell polarization significantly changes calculated transition probability values. Such a behavior is not observed for the remaining transitions. Transition probabilities from the levels 20 and 26 determined in the GK_{CV} approximation are the only ones from [35] which differ by more than 20% from our QR results.

The comparison of the transition probabilities from [33] with our data gives a different picture. Their percentage deviation k

$$k = \left(\frac{A_{[33]}}{A_{QR}} - 1\right) \cdot 100\% \tag{2}$$

are presented in the last column of table 3. One can see from that table that almost a half of transitions of various types agree within 10%. There is a group of 21 transitions where deviations reach up to 50%. For 9 transitions, the deviations are over 50%. Two E1 transition probabilities from the levels 11 and 24 to the level 1 are quite exceptional because their values differ by three orders of magnitude. Unfortunately these transition probabilities are not given in [35]. It is very difficult to find a reason of such an essential difference. As we have explained before, the main LS contributions in the CI wavefunction expansions for these levels agree nicely. Furthermore, there is quite good agreement of the transition probabilities from the levels 11 and 24 to other lower levels. There is one more point worth mentioning here. If one checks the gf values for these particular transitions 11-1 and 24-1 given in [32], it is evident that they differ by more than one order of magnitude going from one approximation to another. Therefore we conclude that it is necessary to perform an independent calculation in order to find correct answer.

The total M1 and E2 transition probability value $A_{\rm M1} + A_{\rm E2} = 7.65 \times 10^6 {\rm s}^{-1}$ is given in [10]. This value agrees very well with our QR value $A_{\rm M1} + A_{\rm E2} = 7.67 \times 10^6 {\rm s}^{-1}$.

In the present work we also have determined parameters for the E3 transition from the excited configuration levels to the ground configuration. As it has been demonstrated in [16, 17], this type of the radiative transitions can significantly affect the calculated radiative lifetime τ values of the metastable levels for the tungsten and other ions with the open 4d shell. This feature occur for the level 6 of the investigated W³⁹⁺ ion. When we include the E3 transition from the level 6 to the level 1, it changes the determined lifetime τ value by 10%. That indicates that such a transition can affect calculated branching ratios for the decay of this level.

There exists another level, the level 8, where the M2 transition to the ground configuration influences the calculated radiative lifetime τ value. For all other levels

of the excited configurations $4s^24p^44d$ and $4s4p^6$, the radiative lifetimes are well-determined by the E1, M1 and E2 transitions. We have no doubt that calculation of the M2 and E3 radiative transitions to the ground configurations is also important for the excited configuration levels of the ions with the open $4p^N$ shell.

4. Summary and conclusions

The developed quasirelativistic approach facilitate multiconfiguration calculations employing the broad CI wavefunction basis of the admixed configurations. For the inclusion of the correlation effects, the transformed radial orbitals are employed. The effectiveness of this approach have been proved in many previous calculations. We include almost 1000 configurations in the CI wavefunction expansion for the excited configurations with the reduced number of CSFs exceeding 400 000.

The admixed configurations are generated by the virtual excitation of electrons from the external 4l and from the inner 3l shells. This leads to the efficient inclusion of the correlation effects. As a result, the calculated level energies for the excited configurations $4s^24p^44d$ and $4s4p^6$ agree very well with the experimental data.

Determined parameters of the radiative E1 transitions agree well with the most reliable relativistic calculations. That makes us to believe that the transition probability values for other considered transitions are accurate enough. Produced QR data make a complete set for three investigated configurations. Hence they can be applied both for the interpretation of new experimental results and for modeling spectra of hightemperature plasma.

We have demonstrated that the E3 radiative transitions along with the M2 transitions to the ground configuration $4s^24p^5$ must be included in order to determine the correct radiative lifetime values for the metastable levels of the excited configurations $4s^24p^44d$ and $4s4p^6$. This conclusion bears similarity with the outcome from our investigation of the multicharged ions with the open 4d shell.

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